Computer Aided Mixing Modeling Using the Galerkin Least-Squares Finite Element Technique.

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A novel approach for computer aided modeling and optimizing mixing process has been developed using Galerkin least-squares finite element technology. Computer aided mixing modeling and analysis involves Lagrangian and Eulerian analysis for relative fluid stretching and energy dissipation concepts for laminar and turbulent flows. High quality, conservative, accurate, fluid velocity and continuity solutions are required for determining mixing quality.

The ORCA Computational Fluid Dynamics (CFD) package, based on a finite element formulation, solves the incompressible Reynolds Averaged Navier Stokes (RANS) equations. Though finite element technology has been well used in areas of heat transfer, solid mechanics, and aerodynamics for years, it has only recently been applied to the area of fluid mixing. Most commercial technologies solve the resultant Partial Differential Equations (PDE's) as discretized approximate solutions using finite volume or finite difference formulations. ORCA has been developed using the Galerkin Least-Squares (GLS) finite element technology. The GLS finite element technique presented provides another formulation for numerically solving the RANS based and LES based fluid mechanics equations.

The Galerkin finite element formulation provides the basis of the formulation but is insufficient to yield a stable solution for the incompressible Navier-Stokes equations. This formulation has its roots in the work of Hughes et al. (1989) and Shakib (1989). Instabilities in the finite element formulation arise from the continuity equation and the convective term in the momentum equations. However, least-squares operators are added providing rigorous mathematical stability and convergence without sacrificing accuracy. The GLS finite element technology is a central difference operator that uses weighted residual formulations for momentum, energy and turbulence equations. This formulation minimizes the error of the approximating functions, while satisfying the all conservation equations (continuity, energy, momentum) locally on the elements and globally on the entire system, and maintaining system stability. Conservation principles are specifically formulated and solved. The GLS formulation provides the basis of the confidence, robustness, accuracy, convergence, and stability of ORCA providing higher order accuracy with respect to the spatial discretization, and 2nd accuracy order in time.

This GLS finite element technique has been extensively validated for both laminar and turbulent mixing and flow problems. Two validation studies are presented to demonstrate the accuracy of the GLS finite element technology for use in fluids mixing.

The GLS finite element method was and experimentally validated, for a stirred tank operated in the laminar regime.. The experimental configuration consisted of three impeller Rushton turbine system experimentally validated for Reynolds Numbers of 20, 40, 80, and 160 (Zalc et al. 2001). This study reveals corresponding quantitative velocity fields, as well as corresponding areas of unmixedness through Poincarè sections, in both results. The

comparison has good qualitative and quantitative agreement between the experimental data and the CFD results.

Having validated the computational approach over a wide range of flow conditions, other scenarios are numerically tested with a high degree of confidence. This will provide insight in to the stirred tank reactor without having to complete a series of time-consuming experimentation.

Compared in detail are a CFD turbulent flow field validation of an axis-symmetric free jet expelled into a stagnant fluid and a fully baffled system mixed with a Rushton turbine system.

ROUND FREE JET

Before any complicated geometry can be modeled, a simple round free jet is modeled. The decay rate and similarity profile can be derived from the Navier-Stokes equations. To compute the CFD properties for a free round jet, an unstructured tetrahedral mesh was used. The CFD parameters are shown in Table 1 and Figure 1 is an indication of the mesh used for this study.

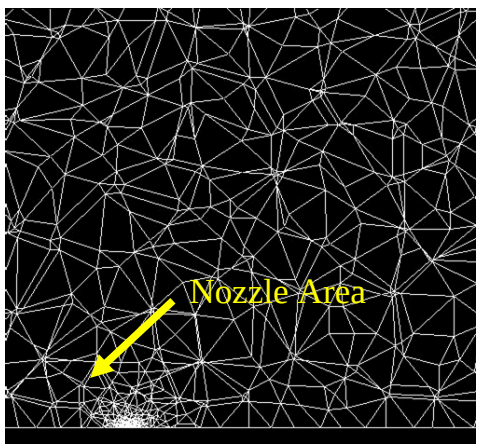

Figure 1: This is a close up of the unstructured tetrahedral mesh used to compute the CFD properties for a free round jet.

<u>Table 1: Parameters for CFD round jet solution</u>

Dimensional Properties

- Nozzle Diameter=0.005m
- Nozzle Velocity=1 m/s
- Fluid=Water

CFD Properties

- Solution time = 2 hours: (on two parallel machines with 900MHz Athlon processors and 512MB ram)
- Solution Tolerance = 10^{-3}
- Turbulence Model = Spalart Allmaras
- Mesh = 1.3 Million Unstructured Tetrahedral Mesh

The similarity profile and the decay rate were examined to determine the predictability of the CFD code. Figure 2 shows the similarity profile of the jet, which has good agreement with the ideal similarity solution profiles from Goertler (1942) similarity profile. Figure 3

indicates the velocity decay of the jet. It shows excellent agreement with the ideal decay rate, with a variance within 1%.

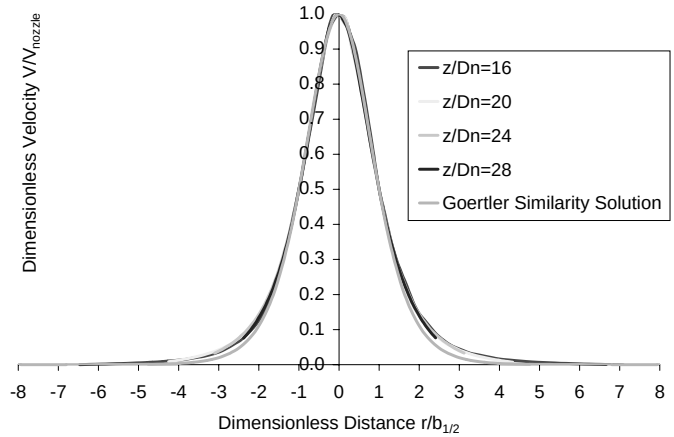

Figure 2: Similarity profile for the free round jet as compared to the Goertler (1942) Similarity Solution. Values compare well with the ideal similarity solution.

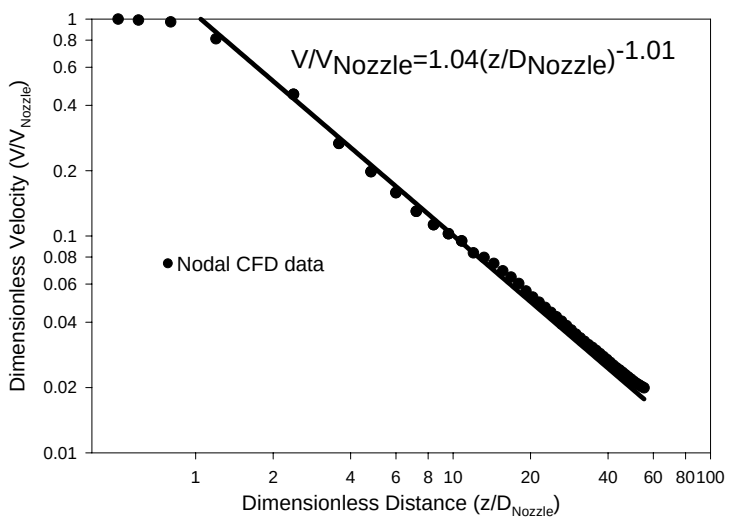

Figure 3: The center line velocity decay of the round jet. The computed decay rate exponent agrees within 1% with the ideal decay rate. This variation is likely associated with the discretization and achieved convergence levels.

Based upon the results of the free jet decay prediction using an unstructured tetrahedral mesh, the examination into more complicated flows can be made with some confidence.

TWO-DIMENSIONAL WALL JETS IN A STIRRED TANK

In CFD/Experimental comparisons of a flow along the wall of the tank, the examination of these flows provide excellent test areas because they mimic 2D jets (Kresta et al. 2001). CFD simulations that could quantitatively predict the wall jet properties would provide an indication that the CFD can be used for more predictive work (i.e., for prediction of the cloud height in a high concentration solids suspension). Bittorf and Kresta (2002) use wall jet properties to predict the cloud height of solid suspensions in stirred tanks. CFD simulations such as these are potentially instrumental in solving engineering problems.

The velocity decay for the wall jet expands and decays ideally, providing the test case for flow field validation for a system mixed with a Rushton Turbine impeller. Table 2 indicates the CFD parameters used, while Figure 4 indicates the location of the two dimensional wall jet in a stirred tank. The two dimensional wall jets are along the wall of the tank and act ideally like an internal annular wall jet. The decay rate and the similarity profile for a wall jet in a recirculating flow as derived from the Navier stokes equations is as follows (Kresta et al. 2001 and Bittorf 2000):

$$\frac{V}{V_{max}} = A\left(\frac{z}{T}\right)^{-0.5} \qquad (1a)$$

$$\frac{V}{V_m} = 1 - 1.75\tanh^2\left[0.702\left(\frac{y}{b_{1/2}}\right) - 0.15\right] \qquad (1b)$$

Table 2: Parameters for CFD round jet solution

Dimensional Properties

- Impeller Diameter, D = 80mm
- Tank Diameter, T = 240 mm
- Impeller Clearance, C = 60mm
- Impeller Speed 500RPM
- Fluid = Water

CFD Properties

- Solution time = 3 hours: (on three parallel machines with 900MHz Athlon processors and 512MB ram)
- Solution Tolerance = 10^{-3}
- Turbulence Model = Spalart Allmaras
- Mesh = 3 Million Unstructured Tetrahedral Mesh

This similarity profile for the jet within a recirculating flow (Kresta et al. 2001 and Bittorf 2000) accounts for the recirculating flow that occurs in a stream that flows up along the wall and downward in the center .

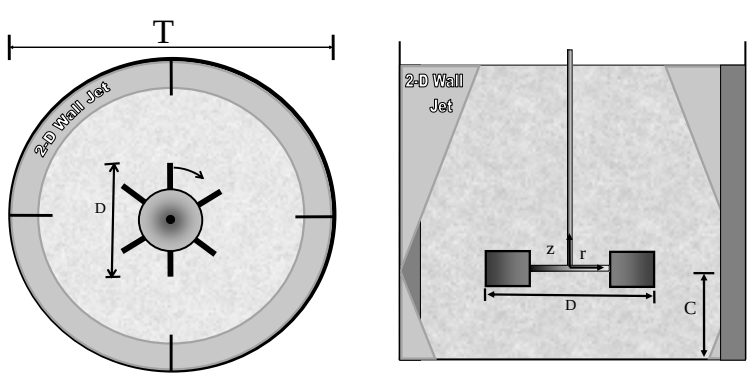

Figure 4: Location of the two Dimensional wall jets in a stirred tank mixed with a Rushton turbine impeller blade.

The two main characteristics examined are the similarity profile and the jet decay as compared to equation 1a and 1b. Figure 5 indicates the similarity profile as compared to Equation 1b. The profiles agree well with some deviation in the recirculation zone. This is encouraging considering the chaotic nature of a stirred vessel.

The CFD data for the decay of the local maximum velocity, presented in Figure 6, shows good agreement between both experimental and theoretical values when compared to the ideal decay of Equation 1a.

The final characteristic examined is the expansion of the jet. As derived from the RANS equations, the half width of the jet ($b_{1/2}$) expands linearly as indicated in Bittorf (2000). The expansion rate calculated from the CFD is 13°, which closely parallels an experimental value of 11° demonstrated by Kresta et al. (2001).

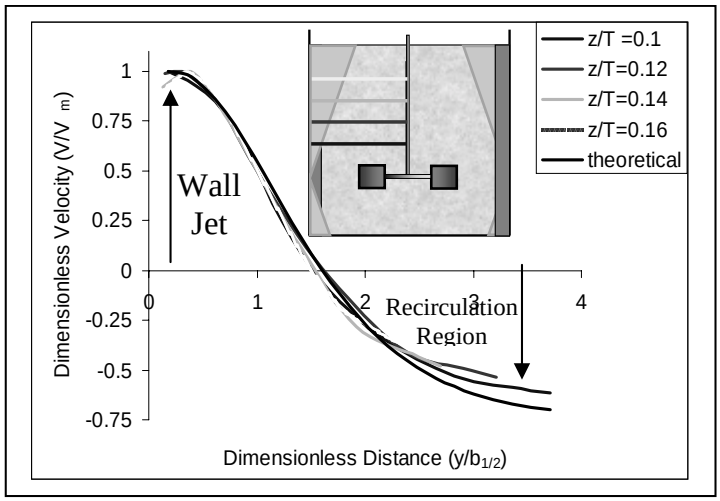

Figure 5: Similarity for an internal annular wall jet with recirculation created by the swirling radial jet from a Rushton turbine. The wall jet region and recirculation region shown in the figure agree well with the theoretical prediction. The x-axis represents the distance from the wall, y, made dimensionless with the half width of the jet, $b_{1/2}$; the y-axis represents the dimensionless velocity.

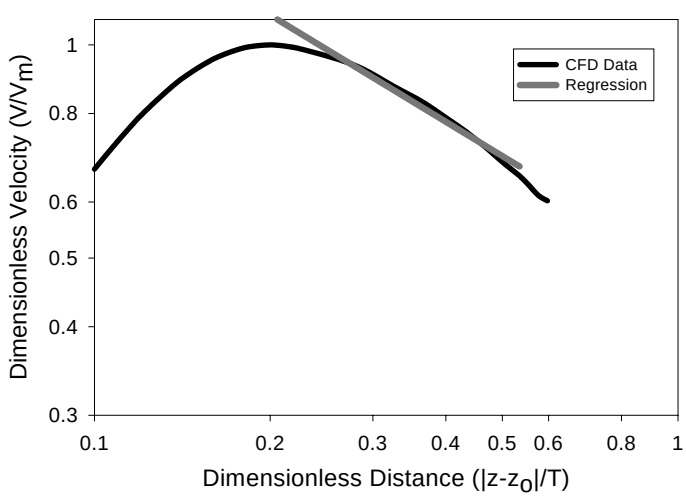

Figure 6: CFD Velocity Decay Rate Predictions for the internal annular wall jet. The CFD matches the theoretical radial decay rate exponent of -0.50 from Kresta [3].

A similar study was completed for three-dimensional wall jets created by axial impeller stirred tanks (Johnson and Bittorf, 2002 and Bhattacharya and Kresta, 2002). Johnson and Bittorf were able to predict the decay rate of the jet and other similarity properties using the GLS finite element method solved with the Spalart-Allmaras turbulence model. While Bhattacharya and Kresta (2002) were able to predict some properties of the jet, there were not able to predict the decay rate of the jet. They used a finite volume solver and variations of the k-ε turbulence and the Reynolds stress models. Because of this, the deviations are likely attributed to one of these factors. Without a direct comparison it is difficult to determine which factors drive the deviation from the ideal decay rate.

CONCLUSION

In conclusion, the GLS finite element formulation presented provides numerical results that agree well with ideal values for a round free jet. As well, the finite element formulation provides a robust and accurate CFD solution for stirred tank velocity fields. These results provide confidence that this method can be a useful tool for engineers involved in solving mixing problems.

Nomenclature

A	Constant
$b_{1/2}$	jet half width (m)
C	impeller clearance (m)
D	impeller diameter (m)
H	tank height (m)
r	radial position (m)
T	tank diameter (m)
V	axial velocity (m/s)
V_m	local maximum velocity (m/s)
V_{max}	absolute maximum velocity (m/s)
y	distance from tank wall (m)
z	axial position (m)

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